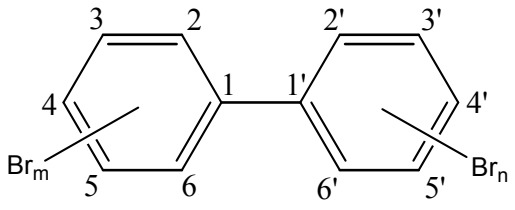
4. CHEMICAL AND PHYSICAL INFORMATION

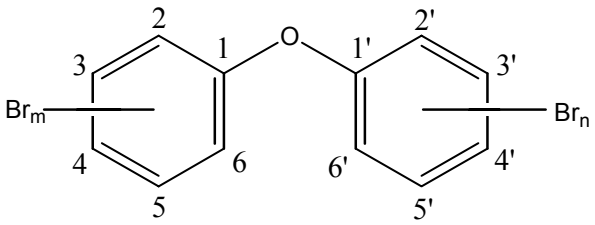
4.1 CHEMICAL IDENTITY

Polybrominated biphenyls (PBBs) and polybrominated diphenyl ethers (PBDEs) are each classes of structurally similar brominated hydrocarbons. PBBs are a class of chemical compounds in which 2–10 bromine atoms are attached to the biphenyl molecule. PBDEs are a class of chemical compounds in which 2–10 bromine atoms are attached to the diphenyl ether molecule. Monobrominated structures (i.e., one bromine atom attached to the molecule) are often included when describing PBBs and PBDEs. The general chemical structures of PBBs and PBDEs are similar when viewed in one dimension, differing only in an ether linkage, as shown below:



where m + n = 1 to 10

PBBs



where m + n = 1 to 10

PBDEs

It can be seen from the structures that a large number of brominated compounds are possible. The 209 possible compounds for both PBBs and PBDEs are called “congeners”. PBBs and PBDEs can also be categorized by degree of bromination. The term “homolog” is used to refer to all PBBs and PBDEs with the same number of bromines (e.g., tribromobiphenyls and tribromodiphenyl ether). Based on the number of bromine substituents, there are 10 homologous groups of PBBs and PBDEs (monobrominated through decabrominated). Each homologous group contains one or more congeners. The mono-, di-, tri-, tetra-, penta-, hexa-, hepta-, octa-, nona-, and decabromo-congeners can exist in 3, 12, 24, 42, 46, 42, 24, 12, 3, and 1 forms, respectively. Homologs with different substitution patterns are referred to as isomers. For example, the dibromobiphenyl and dibromodiphenyl ether homologs both contain 12 isomers. The numbering system for PBBs and PBDEs are also shown above. Positions 2, 2', 6, and 6' are called *ortho* positions, positions 3, 3', 5, and 5' are called *meta* positions, and positions 4 and 4' are called *para* positions. In a PBB molecule, the benzene rings can rotate around the bond connecting them; the two extreme configurations are planar (the two benzene rings are in the same plane; dihedral angle=0E) and nonplanar (the two benzene rings are in perpendicular planes to each other; dihedral angle=90E). The

degree of planarity is largely determined by the number of substitutions in the *ortho* positions. The replacement of hydrogen atoms in the *ortho* positions with larger bromine atoms forces the benzene rings to adopt configuration with a larger dihedral angle or nonplanar configuration. The benzene rings of non-*ortho* substituted PBBs, as well as mono-*ortho* substituted PBBs, may assume a small dihedral angle (in which the dihedral angle is small, but >0E) or "near" planar configuration. These molecules are referred to as planar or coplanar congeners. The benzene rings of other congeners cannot assume a planar or coplanar configuration and are referred to as nonplanar congeners. In contrast, the benzene rings in a PBDE molecule do not rotate freely around the ether linkage connecting them due to a high barrier to rotation resulting from a 120E bend at the ether linkage and steric effects due to the large size of bromine atoms. As a consequence, PBDEs do not assume planar dioxin-like configurations (Hardey 2002).

Like PCBs, the 209 congeners for PBBs and PBDEs are arranged in ascending numerical order using a numbering system developed by Ballschmiter and Zell (1980) that follow the IUPAC rules of substituent characterization in biphenyls. The resulting numbers, also referred to as congener, IUPAC, or BZ numbers, are widely used for identifying individual congeners of PBBs and PBDEs. For example, the PBB congener, 2,2',4,4',5,5'-hexabromobiphenyl, may be referred to as BB-153 in this document. Likewise, the PBDE congener, 2,2',4,4'-tetrabromodiphenyl ether may be referred to as BDE-47 in this document. The identities of several PBB and PBDE congeners are shown in Table 4-1 (WHO 1994a, 1994b).

Polybrominated Biphenyls. Michigan Chemical Corporation, the major producer of PBBs from 1970 to 1976, marketed mixtures of PBBs under the trade name FireMaster (e.g., BP-6 and FF-1). Other producers of PBBs in the United States included White Chemical Corporation (Bayonne, New Jersey) and Hexcel Corporation (Sayreville, New Jersey), which both produced technical mixtures of octabromobiphenyl and decabromobiphenyl until 1979. The trade names of some commercial PBB mixtures formerly produced in other countries are Berk Corporation, Great Britain (e.g., BerkFlam, Flammex), Chemische Fabrik Kalk, Germany (e.g., Bromkal), and Ugine Kuhlmann (now Atofina in France) (e.g., Adine).

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners

		CAS No.[a]	
IUPAC No.[b]	Compound/ substituents	Brominated biphenyls (BB)[c]	Brominated diphenyl ethers (BDE)[d]
	Biphenyl	92-52-4	92-52-4
	Monobromo-	26264-10-8	101-55-3
1	2	2052-07-7	
2	3	2113-57-7	
3	4	92-66-0	
	Dibromo-	27479-65-8	2050-47-7
4	2,2N	13029-09-9	
5	2,3	115245-06-2	
6	2,3N	49602-90-6	
7	2,4	53592-10-2	
8	2,4N	49602-91-7	
9	2,5	57422-77-2	
10	2,6	59080-32-9	
11	3,3N	16400-51-4	
12	3,4	60108-72-7	
13	3,4N	57186-90-0	
14	3,5	16372-96-6	
15	4,4N	92-86-4	
	Tribromobiphenyl	51202-79-0	49690-94-0
16	2,2’,3		
17	2,2’,4		
18	2,2N,5	59080-34-1	
19	2,2’,6		
20	2,3,3’		
21	2,3,4		
22	2,3,4’		
23	2,3,5		
24	2,3,6		
25	2,3’,4		
26	2,3N,5	59080-35-2	
27	2,3’,6		
28	2,4,4N	6430-90-6	
29	2,4,5	115245-07-3	
30	2,4,6	59080-33-0	

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners *(continued)*

		CAS No.[a]	
IUPAC No.[b]	Compound/ substituents	Brominated biphenyls (BB)[c]	Brominated diphenyl ethers (BDE)[d]
31	2,4N,5	59080-36-3	
32	2,4N,6	64258-03-3	
33	2',3,4		
34	2',3,5		
35	3,3',4		
36	3,3',5		
37	3,4,4N	6683-35-8	
38	3,4,5	115245-08-4	
39	3,4N,5	72416-87-6	
	Tetrabromobiphenyl	40088-45-7	40088-47-9
40	2,2',3,3'		
41	2,2',3,4		
42	2,2',3,4'		
43	2,2',3,5		
44	2,2',4,5'		
45	2,2',3,6		
46	2,2',3,6'		
47	2,2N,4,4'	66115-57-9	
48	2,2',4,5		
49	2,2N,4,5'	60044-24-8	
50	2,2',4,6		
51	2,2N,4,6'	97038-95-4	
52	2,2N,5,5'	59080-37-4	
53	2,2N,5,6'	60044-25-9	
54	2,2N,6,6'	97038-96-5	
55	2,3,3N,4	97038-99-8	
56	2,3,3',4'		
57	2,3,3',5		
58	2,3,3',5'		
59	2,3,3',6		
60	2,3,4,4'		
61	2,3,4,5	115245-09-5	
62	2,3,4,6	115245-10-8	
63	2,3,4',5		
64	2,3,4',6		
65	2,3,5,6		

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners *(continued)*

		CAS No.[a]	
IUPAC No.[b]	Compound/ substituents	Brominated biphenyls (BB)[c]	Brominated diphenyl ethers (BDE)[d]
66	2,3N,4,4N	84303-45-7	
67	2,3',4,5		
68	2,3',4,5'		
69	2,3',4,6		
70	2,3N,4N,5	59080-38-5	
71	2,3',4',6		
72	2,3',5,5'		
73	2,3',5',6		
74	2,4,4',5		
75	2,4,4N,6	64258-02-2	
76	2',3,4,5		
77	3,3N,4,4N	77102-82-0	
78	3,3',4,5		
79	3,3N,4,5N	97038-98-7	
80	3,3N,5,5N	16400-50-3	
81	3,4,4N,5	59589-92-3	
	Pentabromobiphenyl	56307-79-0	32534-81-9
88	2,2N,3,4,6	77910-04-4	
89	2,2',3,4,6'		
90	2,2',3,4',5		
91	2,2',3,4',6		
92	2,2',3,5,5'		
93	2,2',3,5,6		
94	2,2',3,5,6'		
95	2,2N,3,5N,6	88700-05-4	
96	2,2',3,6,6'		
97	2,2',3',4,5		
98	2,2',3',4,6		
99	2,2N,4,4N,5	81397-99-1	
100	2,2N,4N,4N,6	97038-97-6	
101	2,2N,4,5,5N	67888-96-4	
102	2,2N,4,5,6N	80274-92-6	
103	2,2N,4,5N,6	59080-39-6	
104	2,2N,4,6,6N	97063-75-7	
105	2,3,3',4,4'		
106	2,3,3',4,5		
107	2,3,3',4',5		

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners *(continued)*

IUPAC No.[b]	Compound/ substituents	CAS No.[a] Brominated biphenyls (BB)[c]	CAS No.[a] Brominated diphenyl ethers (BDE)[d]
108	2,3,3',4,5'		
109	2,3,3',4,6		
110	2,3,3',4',6		
111	2,3,3',5,5'		
112	2,3,3',5,6		
113	2,3,3',5',6		
114	2,3,4,4N,5	96551-70-1	
115	2,3,4,4',6		
116	2,3,4,5,6	38421-62-4	
117	2,3,4',5,6		
118	2,3N,4,4N,5	6788-97-5	
119	2,3N,4,4N,6	86029-64-3	
120	2,3N,4,5,5N	80407-70-1	
121	2,3',4,5',6		
122	2',3,3',4,5		
123	2N,3,4,4N,5	74114-77-5	
124	2',3,4,5,5'		
125	2',3,4,5,6'		
126	3,3N,4,4N,5	84303-46-8	
127	3,3N,4,5,5N	81902-33-2	
	Hexabromobiphenyl	36355-01-8	36483-60-0
128	2,2N,3,3N,4,4N	82865-89-2	
129	2,2'3,3',4,5		
130	2,2N,3,3N,4,5N	82865-90-5	
131	2,2',3,3',4,6		
132	2,2N,3,3N,4,6N	119264-50-5	
133	2,2N,3,3N,5,5N	55066-76-7	
134	2,2',3,3',5,6		
135	2,2N,3,3N,5,6N	119264-51-6	
136	2,2',3,3',6,6'		
137	2,2N,3,4,4N,5	81381-52-4	
138	2,2N,3,4,4N,5N	67888-98-6	
139	2,2',3,4,4',6		
140	2,2',3,4,4',6		
141	2,2N,3,4,5,5N	120991-47-1	
142	2,2',3,4,5,6		
143	2,2',3,4,5,6'		

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners *(continued)*

IUPAC No.[b]	Compound/ substituents	CAS No.[a] Brominated biphenyls (BB)[c]	CAS No.[a] Brominated diphenyl ethers (BDE)[d]
144	2,2N,3,4,5N,6	119264-52-7	
145	2,2',3,4,6,6'		
146	2,2',3,4',5,5'		
147	2,2',3,4',5,6		
148	2,2',3,4',5,6'		
149	2,2N,3,4N,5N,6	69278-59-7	
150	2,2N,3,4N,5,6N	93261-83-7	
151	2,2N,3,5,5N,6	119264-53-8	
152	2,2',3,5,6,6'		
153	2,2N,4,4N,5,5N	59080-40-9	
154	2,2N,4,4N,5,6N	36402-15-0	
155	2,2N,4,4N,6,6N	59261-08-4	
156	2,3,3N,4,4N,5	77607-09-1	
157	2,3,3N,4,4N,5N	84303-47-9	
158	2,3,3',4,4',6		
159	2,3,3N,4,5,5N	120991-48-2	
160	2,3,3',4,5,6		
161	2,3,3',4,5',6		
162	2,3,3',4',5,5'		
163	2,3,3',4',5,6		
164	2,3,3N,4N,5N,6	82865-91-5	
165	2,3,3',5,5',6		
166	2,3,4,4',5,6		
167	2,3N,4,4N,5,5N	67888-99-7	
168	2,3N,4,4N,5N,6	84303-48-0	
169	3,3N,4,4N,5,5N	60044-26-0	
	Heptabromobiphenyl	35194-78-6	68928-80-3
170	2,2N,3,3N,4,4N,5	69278-60-0	
171	2,2',3,3',4,4',6		
172	2,2N,3,3N,4,5,5N	82865-92-7	
173	2,2',3,3',4,5,6		
174	2,2N,3,3N,4,5,6N	88700-04-3	
175	2,2',3,3',4,5',6		
176	2,2',3,3',4,6,6'		
177	2,2',3,3',4,5,6'		
178	2,2N,3,3N,5,5N,6,	119264-54-9	
179	2,2',3,3',5,6,6'		

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners *(continued)*

IUPAC No.[b]	Compound/ substituents	CAS No.[a] Brominated biphenyls (BB)[c]	CAS No.[a] Brominated diphenyl ethers (BDE)[d]
180	2,2N,3,4,4N,5,5N	67733-52-2	
181	2,2',3,4,4',5,6		
182	2,2N,3,4,4N,5,6N	119264-55-0	
183	2,2',3,4,4',5',6		
184	2,2N,3,4,4N,6,6N	119264-56-1	
185	2,2',3,4,5,5',6		
186	2,2N,3,4,5,6,6N	119264-57-2	
187	2,2N,3,4N,5,5N,6	84303-49-1	
188	2,2N,3,4N,5,6,6N	119264-58-3	
189	2,3,3N,4,4N,5,5N	88700-06-5	
190	2,3,3N,4,4N,5,6	79682-25-0	
191	2,3,3',4,4',5',6		
192	2,3,3',4,5,5',6		
193	2,3,3',4',5,5',6		
	Octabromobiphenyl	27858-07-7	32536-52-0
194	2,2N,3,3N,4,4N,5,5N	67889-00-3	
195	2,2',3,3',4,4',5,6		
196	2,2',3,3',4,4',5',6		
197	2,2N,3,3N,4,4N,6,6N	119264-59-4	
198	2,2',3,3',4,5,5',6		
199	2,2',3,3',4,5,6,6'		
200	2,2N,3,3N,4,5,6,6N	119264-60-7	
201	2,2N,3,3N,4,5N,6,6N	69887-11-2	
202	2,2N,3,3N,5,5N,6,6N	59080-41-0	
203	2,2',3,4,4',5,5',6		
204	2,2N,3,4,4N,5,6,6N	119264-61-8	
205	2,3,3',4,4',5,5',6		
	Nonabromobiphenyl	27753-52-2	63936-56-1
206	2,2N,3,3N,4,4N,5,5N,6	69278-62-2	
207	2,2N,3,3N,4,4N,5,6,6N	119264-62-9	
208	2,2N,3,3N,4,5,5N,6,6N	119264-63-0	

Table 4-1. Chemical Identity of Polybrominated Biphenyl (PBB) and Polybrominated Diphenyl Ether (PBDE) Congeners *(continued)*

IUPAC No.[b]	Compound/ substituents	CAS No.[a] Brominated biphenyls (BB)[c]	CAS No.[a] Brominated diphenyl ethers (BDE)[d]
	Decabromobiphenyl	13654-09-6	1163-19-5
209	2,2N,3,3N,4,4N,5,5N,6,6N	13654-09-6	1163-19-5

[a]Not all of PBBs have been assigned CAS numbers; with the exception of BDE-209, no CAS numbers were identified for the PBDE class.
[b]Ballschmiter and Zell 1980
[c]WHO 1994b
[d]WHO 1994a

The chemical identity of hexabromobiphenyl, octabromobiphenyl, decabromobiphenyl (BB-209), and 2,2',4,4',5,5'-hexabromobiphenyl (BB-153), the most abundant congener in commercial FireMaster FF-1 and FireMaster BP-6, are listed in Table 4-2.

Polybrominated Diphenyl Ethers. In the United States, Albemarle Corporation and Great Lakes Chemical Corporation market mixtures of PBDEs under trade names (e.g., Bromkal 70-5DE, DE-71, Tardex 50, Tardex 50 L, and Saytex 115 for pentaBDE mixtures; DE-79, FR-1208, and Saytex 111 for octaBDE mixtures; and DE 83, FR-300 BA, and Saytex 102 for decaBDE mixtures). The are also several trade names used by producers from Europe and Japan for the BDE mixtures. The chemical identities of commercial mixtures of pentaBDE, octaBDE, and decaBDE are listed in Table 4-3 (WHO 1994a).

Various synonyms and abbreviations for polybrominated diphenyl ethers exist in the literature and are shown below:

polybrominated biphenyl ethers	/ polybromobiphenyl ethers	/ PBBEs
polybrominated biphenyl oxides	/ polybromobiphenyl oxides	/ PBBEs
polybrominated diphenyl ethers	/ polybromodiphenyl ethers	/ PBDEs or PBDPEs
polybrominated diphenyl oxides	/ polybromodiphenyl oxides	/ PBDOs or PBDPOs

For consistency in this document, polybrominated diphenyl ethers or PBDEs will be used to identify this class of chemicals. The PBDE homologs are abbreviated as follows in this document:

Dibromodiphenyl ether	/	DiBDE	/	diBDE
Tribromodiphenyl ether	/	TrBDE	/	triBDE
Tetrabromodiphenyl ether	/	TeBDE	/	tetraBDE
Pentabromodiphenyl ether	/	PeBDE	/	pentaBDE
Hexabromodiphenyl ether	/	HxBDE	/	hexaBDE
Heptabromodiphenyl ether	/	HpBDE	/	heptaBDE
Octabromodiphenyl ether	/	OBDE	/	octaBDE
Nonabromodiphenyl ether	/	NoBDE	/	nonaBDE
Decabromodiphenyl ether	/	DeBDE	/	decaBDE

Table 4-2. Chemical Identity of Selected PBBs[a]

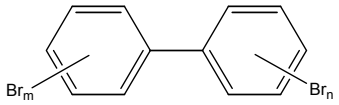
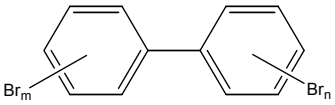
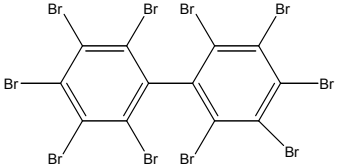
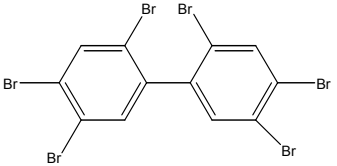
Characteristic	Hexabromobiphenyl	Octabromobiphenyl	Decabromobiphenyl	2,2',4,4'5,5'-Hexabromo-biphenyl
Synonym(s)	FireMaster BP-6[b]; FireMaster FF-1[b]	Bromkal 80[b]	Flammex B 10[b]; Adine 0102[b]; Berkflam B 10[b]	2,2',4,4'5,5'hexabromo-1,1'-biphenyl
Registered trade name(s)	FireMaster BP-6; FireMaster FF-1	Bromkal 80	Flammex B 10; Adine 0102; Berkflam B 10	None
Chemical formula	$C_{12}H_4Br_6$	$C_{12}H_2Br_8$	$C_{12}Br_{10}$	$C_{12}H_4Br_6$
Chemical structure	 m+n = 6	 m + n = 8		
Identification numbers:				
CAS registry	59536-65-1 (BP-6); 67774-32-7 (FF-1); 36355-01-8 (hexabromo mixture)	27858-07-7 (octobromo mixture) 61288-13-9 (Bromkal 80)	13654-09-6 (pure and technical)	59080-40-9
NIOSH RTECS[c]	LK 5060000 (BP-6); LK 5065000 (FF-1)	DV 570000 (octabromo mixture)	No data	No data
EPA hazardous waste	No data	No data	No data	No data
OHM/TADS	No data	No data	No data	No data
DOT/UN/NA/IMCO shipping	No data	No data	No data	No data
HSDB	No data	No data	No data	No data

Table 4-2. Chemical Identity of Selected PBBs[a]

Characteristic	Hexabromobiphenyl	Octabromobiphenyl	Decabromobiphenyl	2,2',4,4'5,5'-Hexabromo-biphenyl
NCI	No data	No data	No data	No data

[a]All information obtained from IARC 1986 except where noted
[b]These are mixtures of compounds, and their compositions are given in the text.
[c]RTECS

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

Table 4-3. Chemical Identity of Selected Technical PBDEs

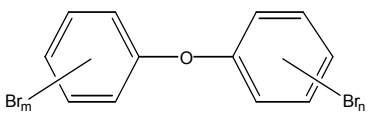
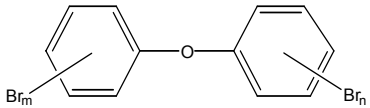
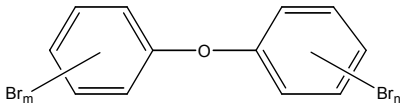
Characteristic	Pentabromodiphenyl ether	Octabromodiphenyl ether	Decabromodiphenyl ether
Synonym(s)	Pentabromodiphenyl ether; pentabromodiphenyl oxide; pentabromobiphenyl oxide; benzene, 1,1-oxybis, pentabromo derivative	Octabromodiphenyl ether; octabromodiphenyl oxide; octabromobiphenyl oxide; benzene, octabromo derivative; phenyl ether, octabromo derivative	Decabromodiphenyl ether; decabromodiphenyl oxide; decabromobiphenyl oxide; benzene, 1,1'-oxybis(2,3,5,6,-penta-bromo-) ether, bis(pentabromophenyl);
Registered trade name	DE 71; Bromkal 70-5 DE; FR 1205/1215; Bromkal 70; Bromkal G1; Pentabromprop; Tardex 50; Tardex 50 L; Saytex 115	Bromkal 7908DE; DE 79; FR 143; Tardex 80; FR 1208; Adine 404; Saytex 111	FR-300 BA; DE-83-RTM; Saytex 102; Saytex 102E; FR-1210; Adine 505; AFR 1021; Berkflam B10E; BR55N; Bromkal 81; Bromkal 82-ODE; Bromkal 83-10 DE; Caliban F/R-P 39P; Caliban F/R-P 44; Chemflam 011; DE 83; DP 10F; EB 10FP; EBR 700; Flame Cut BR 100; FR P-39; BR 100; FR 330BA; FR P-39; FRP 53; FR-PE; FR-PE(H); Planelon DB 100; Tardex 100; NC-1085; HFO-102; Hexcel PF1; Phoscon Br-250
Chemical formula	$C_{12}H_{10-y}Br_yO$ where y = 4 to 6	$C_{12}H_{10-y}Br_yO$ where y = 6 to 9	$C_{12}Br_{10}O$
Chemical structure	 m + n = 4 to 6	 m + n = 6 to 9	 m + n = 10
Identification numbers:			
CAS registry	32534-81-9	32536-52-0	1163-19-5
NIOSH RTECS	No data	No data	No data
EPA hazardous waste	No data	No data	No data

Table 4-3. Chemical Identity of Selected Technical PBDEs *(continued)*

Characteristic	Pentabromodiphenyl ether	Octabromodiphenyl ether	Decabromodiphenyl ether
OHM/TADS	No data	No data	No data
DOT/UN/IMCO shipping	No data	No data	No data
HSDB	No data	No data	No data
NCI	No data	No data	No data

Source: WHO (1994a)

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; PBB = polybrominated biphenyl; RTECS = Registry of Toxic Effects of Chemical Substances

4.2 PHYSICAL AND CHEMICAL PROPERTIES

Polybrominated Biphenyls. Information found in the literature regarding the physical and chemical properties of hexabromobiphenyl, octabromobiphenyl, decabromobiphenyl, and 2,2',4,4',5,5'-hexabromobiphenyl is presented in Table 4-4. The data for the properties listed in Table 4-4 may not be reliable because products of questionable purity were used by earlier investigators to derive them. For example, the water solubility of hexabromobiphenyl (Neufeld et al. 1977) was reported to be the same as that of FireMaster FF-1 (Getty et al. 1977), although FireMaster FF-1 contained only 84.4% (Robertson et al. 1983b) hexabrominated biphenyls.

Of the 209 possible congeners of PBBs, only about 42 have been synthesized in pure form even on a laboratory scale (Sundstrom et al. 1976b). The PBBs produced for commercial use were mixtures of PBBs with other non-PBB impurities. The technical products were FireMaster BP-6, FireMaster FF-1, Bromkal 80, and Flammex B 10 (or Adine 0102 or Berkflam B 10) (IARC 1986). FireMaster FF-1, a white powder, was made by grinding brown flakes of FireMaster BP-6 and adding 2% calcium silicate as an anticaking agent (Fries 1985b). The exact composition of FireMaster BP-6 or FireMaster FF-1 seems to have varied between and within batches (Sundstrom et al. 1976a). Table 4-5 provides the concentrations of the PBB congeners in FireMaster FF-1 and FireMaster BP-6.

An interesting feature of commercial FireMaster FF-1 and FireMaster BP-6 is that they contain >50% of the congener 2,2',4,4',5.5',-hexabromobiphenyl (BB-153). The second most abundant congener is 2,2',3,4,4',5,5'-heptabromobiphenyl (BB-180). A detailed analysis of FireMaster BP-6 (lot 7062) was able to separate 22 congeners of PBBs that included four tri, five tetra, three penta, seven hexa, and three hepta congeners of PBBs (Robertson et al. 1983b, 1984b). The coplanar and toxic congeners 3,3',4,4'-tetra-, 3,3',4,4',5-penta-, and 3,3',4,4',5,5'-hexabrominated biphenyls were found at abundances of 0.159, 0.079, and 0.294%, respectively (Orti et al. 1983; Robertson et al. 1983b). In addition to the 22 congeners, other investigators have identified 2,2',3,3',4,4',5,6'-octa-, 2,2',3,3',4,4',5,5'-octa-, 2,2',3,3',4,4',5,5',6-nona-, and deca-bromobiphenyl in commercial PBBs (Moore et al. 1978). Other impurities detected in FireMaster FF-1 and FireMaster BP-6 were tetra-, penta-, and hexabromonaphthalene (Di Carlo et al. 1978); however, at a detection limit of 0.5 ppm, brominated dioxins and dibenzofurans were not detected in commercial FireMaster FF-1 or FireMaster BP-6 (Hass et al. 1978).

Table 4-4. Physical and Chemical Properties of Selected PBBs[a]

Property	Hexabromobiphenyl	Octabromobiphenyl	Decabromobiphenyl	2,2',4,4',5,5'-Hexabromobiphenyl
Molecular weight	627.4	785.2	943.1	627.4
Color	White	White	White	White
Physical state	Solid	Solid	Solid	Solid
Melting point	72 EC	200–250 EC; 367–367 EC[b] (for industrial product)	380–386 EC	No data
Boiling point	No data	No data	No data	No data
Density	No data	No data	No data	No data
Odor	No data	No data	No data	No data
Odor threshold:				
Water	No data	No data	No data	No data
Air	No data	No data	No data	No data
Solubility:				
Water	11 µg/L	20–30 µg/L	Insoluble	11 µg/L[c]
Organic solvent(s)	Soluble in acetone, benzene	Soluble in methylene chloride, benzene	Moderately soluble in chlorobenzene, *o*-xylene	Acetone (6 weight percent); benzene (75 weight percent)[c]
Partition coefficients:				
Log K_{ow}	6.39[d]	5.53	8.58[e]	9.10 (estimated)[c]
Log K_{oc}	3.33–3.87[f]	No data	No data	5.088[c]
Vapor pressure	5.2×10^{-8} mmHg at 25 EC[g]	7×10^{-11} mmHg at 28 EC[h]	No data	7.6×10^{-5} mm Hg at 90 EC[c]
Henry's law constant	3.9×10^{-6} atm•m^3/mol[i]	No data	No data	5.7×10^{-3} atm•m^3/mol[c]
Autoignition temperature	No data	No data	No data	No data
Flashpoint	No data	No data	No data	No data
Flammability limits	No data	No data	No data	No data

Table 4-4. Physical and Chemical Properties of Selected PBBs[a] *(continued)*

Property	Hexabromobiphenyl	Octabromobiphenyl	Decabromobiphenyl	2,2',4,4',5,5'-Hexabromobiphenyl
Conversion factors	[j]	[j]	[j]	[j]
Explosive limits	No data	No data	No data	No data

[a]All information obtained from IARC (1978) and Norris et al. (1973) unless otherwise noted
[b]Sundstrom et al. 1976
[c]Hardy (2002)
[d]Doucette and Andren 1988
[e]The values for 2,2'4,4'6,6'- and 2,2',3,3',4,4'-hexabromobiphenyl are given as 7.20 (Chessells et al. 1992) and 8.09 (Anliker et al. 1988), respectively.
[f]Estimated from the Freundlich adsorption constants given by Jacobs et al. (1978)
[g]Jacobs et al. 1976
[h]Waritz et al. 1977
[i]Estimated from the ratio of vapor pressure and water solubility
[j]Since these compounds exist in the particle phase in the ambient atmosphere, the concentrations in air are expressed in weight per unit volume of the air.

Table 4-5. Identified PBB Congeners in FireMaster® BP-6 and FireMaster® FF-1

IUPAC No.[a]	Structure	% Composition of FireMaster BP-6	% Composition of FireMaster FF-1	References
Dibromobiphenyls				
4	2,2'-	0.020		Moore et al. 1979
Tribromobiphenyls				
18	2,2',5-	0.050		Robertson et al. 1984
26	2,3',5-	0.024		
31	2,4',5-	0.015		
37	3,4,4'-	0.021		
Tetrabromobiphenyls				
49	2,2',4,5'-	0.025		
52	2,2',5,5'-	0.052		
66	2,3',4,4'-	0.028		
70	2,3',4',5-	0.017		
77	3,3',4,4'-		<0.080	Orti et al. 1983
		0.159		Robertson et al. 1984
Pentabromobiphenyls				
95	2,2',3,5',6-	0.020		Orti et al. 1983
99	2,2',4,4',5-		<0.08	
101	2,2',4,5,5'-	2.69		Robertson et al. 1984
		4.50	3.70	Aust et al. 1981
			1.54	Orti et al. 1983
		2.60		Krüger 1988
118	2,3',4,4',5-	2.94		Robertson et al. 1984
			0.70	Robertson et al. 1984
		3.20		Krüger 1988
126	3,3',4,4',5-		<0.01	
		0.079		Robertson et al. 1984
Hexabromobiphenyls				
132	2,2'3,3',4,6'-	1		Krüger 1988
138	2,2',3,4,4',5'-	12.3		Robertson et al. 1984
		12	8.6	Aust et al. 1981
			5.23	Orti et al. 1983
		10.6		Krüger 1988
149	2,2',3,4',5',6-	2.24		Robertson et al. 1984
		1.40	1.30	Aust et al. 1981
			0.78	Orti et al. 1983

Table 4-5. Identified PBB Congeners in FireMaster® BP-6 and FireMaster® FF-1 *(continued)*

IUPAC No.[a]	Structure	% Composition of FireMaster BP-6	% Composition of FireMaster FF-1	References
153	2,2',4,4',5,5'-	53.9		Robertson et al. 1984
		47.8	47.1	Aust et al. 1981
		55.2		Orti et al. 1983
		58.5		Krüger 1988
155	2,2'4,4',6,6'-	0.5		
156	2,3,3',4,4',5-	0.980		Robertson et al. 1984
		5.0		Aust et al. 1981
		0.37		Orti et al. 1983
		1.0		Krüger 1988
157	2,3,3',4,4',5'-	0.05		Orti et al. 1983
		0.526		Robertson et al. 1984
		0.5`		Krüger 1988
167	2,3',4,4',5,5'-	5.5	3.3	Aust et al. 1981
		3.37		Orti et al. 1983
		<0.3		
		7.95		Robertson et al. 1984
		5.5		Krüger 1988
169	3,3',4,4',5,5'-	0.294		Robertson et al. 1984
Heptabromobiphenyls				
170	2,2',3,3',4,4',5-	0.256		
		1.1	1.5	Aust et al. 1981
		1.66		Orti et al. 1983
		2.4		Krüger 1988
172	2,2',3,3',4,5,5'-	<0.30		Orti et al. 1983
174	2,2',3,3',4,5,6'-	0.24		
178	2,2',3,3',5,5',6-	0.3		Krüger 1988
180	2,2',3,4,4',5,5'	6.97		Robertson et al. 1984
			24.7	Aust et al. 1981
			23.5	Orti et al. 1983
187	2,2',3,4',5,5',6-	0.392		Robertson et al. 1984
			1.0	Krüger 1988
189	2,3,3',4,4',5,5'-		0.51	Orti et al. 1983
Octabromobiphenyls				
194	2,2',3,3',4,4',5,5'-	0.9	2.4	Aust et al. 1981
			1.65	Orti et al. 1983
196	2,2',3,3',4,4',5,6'-			Moore et al. 1980
201	2,2',3,3',4,5,5',6'-			Orti et al. 1983
203	2,2',3,4,4',5,5',6-			

Source: WHO (1994b)

[a]Ballschmiter and Zell (1980)

Commercial octabromobiphenyl (Bromkal 80) contained at least four compounds. Assays of two commercial octabromobiphenyls showed the following compositions: 1.0–1.8% heptabromobiphenyl, 33.0–45.2% octabromobiphenyl, 47.4–60.0% nonabromobiphenyl, and 5.7–6.0% decabromobiphenyl (Norris et al. 1973; Waritz et al. 1977). Notably, the major component of commercial octabromobiphenyl was nonabromobiphenyl, and not octabromobiphenyl. Commercial decabromobiphenyl (Flammex B 10) contained 96.8% decabromobiphenyl, 2.9% nonabromobiphenyl, and 0.3% octabromobiphenyl (Di Carlo et al. 1978).

Pyrolysis of FireMaster BP-6 in the temperature range of 600–900 EC in the absence of oxygen produced bromobenzenes and brominated biphenyls as key products, but no brominated dioxins and dibenzofurans (Thoma and Hutzinger 1987; Thoma et al. 1987). Thermolysis of FireMaster BP-6 between 400 and 600 EC in the presence of air produced 2,3,7,8-tetrabromodibenzofuran in the percent (. 1%=10 g/kg) range (Rappe and Buser 1980). Pyrolysis of FireMaster BP-6 in an open quartz tube at 800 EC produced 0.48–1.49 g/kg 2,3,7,8-TCDD equivalent levels of polybrominated dibenzofurans (Zacharewski et al. 1988). FireMaster BP-6 hydrolyzed when refluxed with 2% potassium hydroxide in ethanol, but the possible rate of PBB hydrolysis under much milder environmental conditions remains unknown (Pomerantz et al. 1978).

Polybrominated Diphenyl Ethers. Information found in the literature regarding the physical and chemical properties of selected technical PBDE mixtures is presented in Table 4-6.

Commercially available product mixtures of PBDEs (see Table 4-3) are not pure substances, but instead are mixtures of congeners. For example, the commercial mixture pentabromodiphenyl ether denotes the main component of the mixture contains the pentabromodiphenyl ether homolog. However, the commercial pentaBDE mixture actually contains tetraBDE (24–38%), pentaBDE (50–62%) homologs with small amounts of hexaBDE (4–8%) and trace amounts of triBDE (0–1%) homologs. In this document, the commercial mixture of pentaBDE will be called “technical pentaBDE” or “technical PeBDE” to distinguish this mixture of homologs from the pentaBDE homolog which refers to polybrominated diphenyl ethers with only five bromine atoms (see Section 4.1). Commercial octabromodiphenyl ether is a mixture of hexa- hepta-, octa-, and nonabrominated diphenyl ether homologs with trace amounts of decabromodiphenyl ether (i.e., BDE-209). In this document, the commercial mixture of octaBDE will be referred to as “technical octaBDE” or “technical OBDE” to distinguish this mixture of different homologs from the octaBDE homolog which refers to

Table 4-6. Physical and Chemical Properties of Technical PBDE Mixtures

Property	Pentabromodiphenyl ether	Octabromodiphenyl ether	Decabromodiphenyl ether
Molecular weight	Mixture	Mixture	959.22[a]
Color	Clear, amber to pale yellow[a]	Off-white[a]	Off-white[a]
Physical state	Highly viscous liquid	Powder	Powder[a]
Melting point:	-7 to -3 EC (commercial)	200 EC (range, 167–257)[a]; 79–87 EC[a]; 170–220 E C[a]	290–306 EC[a]
Boiling point:	>300E C (decomposition starts above 200 EC)[a]	No data	Decomposes at >320, >400, and 425 EC[a]
Density (g/mL)	2.28 at 25 EC[a]	2.76[a]	3.0[a] 3.25[a]
Odor	No data	Faint[a]	Odorless[a]
Odor threshold:			
Water	No data	No data	Not applicable
Air	No data	No data	Not applicable
Solubility:			
Water	13.3 µg/L[b]	<1 g/L at 25 EC[a]	20–30 µg/L at 25 EC[a]
Organic solvent(s)	10 g/kg methanol; miscible in toluene[b]	acetone (20 g/L); benzene (200 g/L); methanol (2 g/L) all at 25 EC[a]	acetone (1 g/L); benzene (4.8 g/L); methanol (1 g/L); all at 25 EC[a]
Partition coefficients:			
Log K_{ow}	6.64–6.97[b]	8.35–8.90[b]	9.97[b]
Log K_{oc}	4.89-5.10[c]	5.92-6.22[c]	6.80[c]
Vapor pressure	$2.2x10^{-7}$ - $5.5x10^{-7}$ mm Hg at 25 EC[b]	$9.0x10^{-10}$-$1.7x10^{-9}$ mm Hg at 25 EC[b]	$3.2x10^{-8}$ mm Hg[d]

Table 4-6. Physical and Chemical Properties of Technical PBDE mixtures *(continued)*

Property	Pentabromodiphenyl ether	Octabromodiphenyl ether	Decabromodiphenyl ether
Henry's Law constant (atm-m^3/mole)	$1.2x10^{-5}$ [e] $1.2x10^{-6}$ [c]; $3.5x10^{-6}$ [c]	$7.5x10^{-8}$ [c]; $2.6x10^{-7}$ [c]	$1.62x10^{-6}$ [e] $1.93x10^{-8}$ [b] $1.2x10^{-8}$ [c]; $4.4x10^{-8}$ [c]
Autoignition temperature	Decomposes above 200 EC[b]	No data	Not applicable[a]
Flashpoint	No data	No data	None
Flammability limits	Not applicable (flame retardant)[b]	No data	Non-flammable[a]
Conversion factors	1 ppm=23.48 mg/m^3 at 20 EC[b]	No data	No data
Explosive limits	None [d]	No data	No data

[a] WHO (1994a)
[b] EU (2001)
[c] estimated values were calculated using EPIWIN v3.10 (EPA 2001)
[d] Hardy (2002)
[e] estimate value calculated using vapor pressure and water solubility values in table.

polybrominated diphenyl ethers with only eight bromine atoms (see Section 4.1). The composition of commercial decabromodiphenyl ether is $97% of the decabromodiphenyl ether (i.e., BDE-209); the remainder is nonabromodiphenyl ether homologs and trace amounts of octabromodiphenyl ether homologs (WHO 1994a). In this document, commercial decabromodiphenyl ether will be referred to as "technical decaBDE" or "technical DeBDE" which represents 97% BDE-209 congener with 3% nona- and octaBDE homolog impurities. The compositions of commercial product mixtures of PBDEs such as technical penta-, octa-, and decaBDE are given in Table 4-7. Trace analysis of these commercial mixtures for 15-different 2,3,7,8-substituted brominate dibenzo-*p*-dioxins and dibenzofurans revealed no detectable amounts of these substances (Hardy 2002).

When pyrolysed up to 900 EC, PBDEs release polybrominated dibenzofurans (PBDFs) and polybrominated-*p*-dioxins (PBDDs) (Buser 1986; EU 2001). The amount of PCDFs and PBDDs formed depends upon the conditions of pyrolysis. For example, 2,3,7,8-tetrabromodibenzofuran in ppm concentrations can be generated during pyrolysis of decabromodiphenyl ether in the temperature range of 400–700 EC (Bieniek et al 1989). PBDFs may also be produced during the pyrolysis of polymers containing PBDEs as flame retardants (Brenner and Knies 1993; Dumler et al 1989. 1990; Lenoir et al 1994).

Table 4-7. Composition of Commercial Brominated Diphenyl Ethers

	PBDE Homologs								
Commercial Mixtures	PBDE[a]	TrBDE	TeBDE	PeBDE	HxBDE	HpBDE	OcBDE	NoBDE	DeBDE
DeBDE								0.3–3%	97–98%
OcBDE					10–12%	43–44%	31–35%	9–11%	0–1%
PeBDE		0–1%	24–38%	50–62%	4–8%				
TeBDE[b]	7.6%	No data	41–41.7%	44.4–45%	6.7%				

Source: WHO (1994a)

[a]Unknown structure
[b]No longer commercially produced

DeBDE=Decabromodiphenyl ether; HpBDE=Heptabromodiphenyl ether; HxBDE=Hexabromodiphenyl ether; NoBDE=Nonabromodiphenyl ether; OcBDE=Octabromodiphenyl ether; PBDE=Polybrominated diphenyl ether; PeBDE=Pentabromodiphenyl ether; TeBDE=Tetrabromodiphenyl ether; TrBDE=Tribromodiphenyl ether